

HPV Robust Summaries and Test Plan

CAS# 86508-42-1 Perfluoro compounds, C5-C18,
Presented for purposes of HPV as **Subcategory “PFC Alkanes”**

Table of Contents

1.0 Description of CAS number	
1.1 Introduction	2
1.2 Identity of Substances and Structural Classification	3
1.3 Summary of Chemical and Physical Properties and Lack of Ecological and Toxicological Effects	4
1.4 Use Pattern	5
2.0 Test Plan	6
3.0 Physical Properties	
3.1 Melting Point	7
3.2 Boiling Point	7
3.3 Relative Density	7
3.4 Vapor Pressure	7
3.5 Octanol/Water Partition Coefficients	8
3.6 Water Solubility	9
3.7 pH and pKa Values	10
3.8 Oxidation-Reduction Potential	10
3.9 Adsorption/Desorption to Soil	10
4.0 Environmental Fate and Pathways	
4.1 Photodegradation	10
4.2 Stability in Water	14
4.3 Biodegradation	14
4.4 Fugacity	15
5.0 Ecotoxicity	
5.1 Acute Toxicity to Fish	17
5.2 Acute Toxicity to Aquatic Invertebrates	18
5.3 Acute Toxicity to Aquatic Plants	20
6.0 Mammalian Toxicity	
6.1 Acute Toxicity	22
6.2 Primary Eye and Skin Irritation	24
6.3 Genotoxicity	26
6.4 Repeat Dose Toxicity	28
6.5 Reproductive Toxicity	32
6.6 Development and Teratogenicity Toxicity	33

1.0 Description of CAS number: Subcategory “PFC Alkanes”

1.1 Introduction

This HPV submission addresses a class of inert perfluorinated compounds (PFCs) covered by a single “generic” CAS# 86508-42-1, defined as “Perfluoro-compounds, C5-C18.” (This “generic” CAS number is listed on the TSCA inventory based on the EPA’s suggestion upon submittal of 3M’s consolidated PMN 82-612 through 82-626.) Many compounds covered by this generic CAS number also have individual CAS numbers.

Data are available on a number of compounds within the generic CAS number for PFCs. For the purposes of HPV, this test plan presents existing data on the “PFC alkanes” subcategory of this generic CAS number. Total volumes of products within this subcategory meet the HPV criteria. A second subcategory within the generic CAS number, identified as “PFC amines”, is presented in another test plan. A third subcategory within the generic CAS number, identified as “PFC ethers”, are not presented because total volumes do not meet HPV criteria.

The chemicals included in this class are described as PFCs and are chemically and biologically inert. They are all fully fluorinated and do not contain functional end-groups. As such, the materials within this class are all chemically and biologically inert. PFCs have high Henry’s constants which dictate their environmental partitioning and, as described in Section 1.3, their low potential for interaction with biological membranes. These same physical characteristics dictate that these inert PFCs have extremely short half-lives in biological systems. The available data on this class of material demonstrate very consistent properties with regard to human health and environmental impact. The commonalities within this class are not surprising given the underlying physical/chemical properties. Together, the available data are ample to represent CAS # 86508-42-1, which includes the alkane and amine subcategories for HPV purposes, and no further testing is proposed.

PFCs are inert fluids composed of a complex combination of organic compounds resulting from the distillation of electrochemically fluorinated (ECF) compounds. This class consists of branched, linear and cyclic perfluorinated hydrocarbons having carbon numbers predominantly in the range of C5-C18 and boiling in the range of approximately 25° C to 255° C (77° F – 491° F). Perfluorinated amine and ether compounds may also be present.

3M manufactures a number of products comprised of PFCs, and markets them subject to rigorous product stewardship because of their photochemical stability and global warming potential. Section 1.2 of this subcategory “alkanes” lists four products, each with its own individual CAS number, that are included under this “generic” CAS number and for which data are presented in this test plan. This listing is not intended to be inclusive of all possible chemicals covered by the generic CAS number. Rather, it represents the PFC products manufactured by 3M that were included in 3M’s 1990 IUR submission and remain in the HPV production thresholds today. Data on these products adequately represent the generic CAS number.

This test plan presents physical property data on each of four PFC products. PFCs are highly volatile and insoluble in water. For the environmental and toxicological HPV endpoints, this

test plan summarizes data from one or more PFC products. Data are available for almost all relevant endpoints, although certain physical property and environmental fate tests are not applicable. Ecotoxicity tests for fish and aquatic invertebrates show no toxicity; aquatic plant testing is deemed unnecessary. Acute toxicity and repeat dose toxicity data are available. An acute oral toxicity test shows no toxicity at any dose tested. Ames testing showed no genotoxicity. Further testing for reproductive or developmental effects is unnecessary and inappropriate given that PFCs are chemically and biologically inert.

The chemical and biological stability of this class of materials also results in very long atmospheric lifetimes. The persistence of these materials in the atmosphere and their global warming potential are the primary consideration for the strict product stewardship associated with the marketing and use of these materials. That stewardship dictates that this class of materials be used in niche applications where there are no other alternatives available on the basis of performance or safety.

1.2 Identity of Substances and Structural Classification

3M manufactures four products that fall within the subcategory “PFC alkanes” of generic CAS # 86508-42-1. As noted above, each of these products also has an individual CAS number, although EPA suggested use of the generic CAS number for inventory reporting for these and other compounds.

The table below shows the composition of each PFC product, identifying the predominant molecule representing at least 50% of the total composition of the product as manufactured by 3M. The balance of each product is comprised of other PFCs with the same and similar number of carbon atoms in branched, linear and/or cyclic structure.

SUBCATEGORY: PFC ALKANES

<u>Product</u>	<u>CAS#</u>	<u>Predominant Molecule</u>	<u>Structural Formula</u>
A	678-26-2	Perfluoropentane (C5)	CF ₃ CF ₂ CF ₂ CF ₂ CF ₃
B	355-42-0	Perfluorohexane (C6)	CF ₃ CF ₂ CF ₂ CF ₂ CF ₂ CF ₃
C	335-57-9	Perfluoroheptane (C7)	CF ₃ CF ₂ CF ₂ CF ₂ CF ₂ CF ₂ CF ₃
D	307-34-6	Perfluorooctane (C8)	CF ₃ CF ₂ CF ₂ CF ₂ CF ₂ CF ₂ CF ₂ CF ₃

1.3 Summary of Chemical and Physical Properties and Lack of Ecological and Toxicological Effects

PFCs are among the least toxic of all known organic chemicals. PFCs don't oxidize or hydrolyze. They have no functional reactive groups. PFCs owe their very low toxicity to the combination of the following properties:

1. Chemical inertness
2. Low solubility in biological media (blood, cell membranes, etc.)
3. High volatility
4. Resistance to biological activation (reductive and oxidative metabolism)

Because PFCs are chemically inert, if inhaled and absorbed they do not react chemically with any biological molecules; they simply partition between blood and various organs and tissues. As PFCs have limited ability to dissolve in biological media, they do not reach appreciable concentrations in the tissues of air-exposed animals. As PFCs are highly volatile chemicals and have high air-blood partition coefficients, any fluorochemical remaining after exposure will be rapidly eliminated in the breath. Consequently, all such PFCs have:

1. Very high rodent LC50s (very low acute toxicity)
2. Very high cardiac sensitization EC50s (very low toxicity)

In fact, most PFCs do not induce narcosis (sleep) or cardiac sensitization at maximum achievable concentration (saturation).

PFCs are neutral molecules and because they are maximally fluorinated, they cannot undergo biological oxidation-reduction reactions to form reactive aldehydes, acid fluorides, radicals or acids that have been associated with several types of toxicity. As PFCs are not reactive directly with biological tissue and PFCs cannot form reactive metabolites, these fluorochemicals have tested negative in bacterial mutagenicity assays. Since PFCs are volatile and have limited water solubility, they also have very low toxicity when tested in fish and daphnia studies. These PFCs do not present any significant hazard to aquatic life.

Consequently, all PFCs that have undergone evaluation by the ACGIH or WEEL committees in the US have been granted an exposure guideline of 1000 ppm 8-hour Time Weighted Average (8-hr TWA). NASA has evaluated the toxicity information associated with PFCs including those that can be used as heat transfer agents and fire extinguishing agents in spacecraft and has established a Space Maximum Allowable Concentration (SMAC) of 11,000 ppm for up to 180 days (24 hours/day). (Chiu-Wing Lam, NASA).

1.4 Use Pattern

PFCs are characterized as very stable, non-toxic liquids that have a very high dielectric and very low solubility for water and other airborne contaminants. These materials are also very insoluble in water. In other words, water does not go into PFCs and PFCs do not go into water. These specialty chemicals are used primarily in the industrial electronics industry for applications that exploit these specific properties. The principal applications include industrial heat transfer in semiconductor processing, electronics testing and solvents for computer disc drive lubrication.

Most applications where PFCs are used are regulated by section 612 of the Clean Air Act, which addresses the acceptability of alternatives for ozone-depleting substances. Based on the long atmospheric lifetime and high global warming potential of this class of materials, EPA regulations specify that PFCs may only be used as replacements for ozone-depleting substances in the regulated sectors where they are the only alternative available on the basis of either performance or safety. 3M follows this same guidance in applying product stewardship principles for supply of PFCs to unregulated sectors.

3M has manufactured PFCs at three sites in the U.S. Process improvements have reduced emissions 40% since 1995. 3M anticipates that installation of abatement technology in the next year will reduce emissions to the environment by approximately 90% compared to the 1995 baseline. Although end-use applications are tightly controlled, emissions to the environment do occur at a very low rate. When emitted during manufacturing or from industrial use, the high Henry's Constant for this class of materials dictates preferential partitioning to the atmosphere.

2.0 HPV Test Plan: Subcategory PFC Alkanes

This chart represents the HPV Test Plan for CAS # 86508-42-1, Perfluoro compounds, C5-C18, **Subcategory PFC Alkanes**. This test plan reflects extensive existing data included in this submission. 3M does not propose additional testing.

Endpoint	Information Available	Acceptable	Testing Needed
Physical Properties			
Melting Point	N/A	Yes	No
Boiling Point	Yes	Yes	No
Relative Density	Yes	Yes	No
Vapor Pressure	Yes	Yes	No
Octanol/Water Partition Coefficients	Yes	Yes	No
Water Solubility	Yes	Yes	No
pH and pKa Values	N/A	N/A	No
Oxidation/Reduction Potential	N/A	N/A	No
Adsorption/Desorption to Soil	N/A	N/A	No
Environmental Fate and Pathways			
Photodegradation	Yes	Yes	No
Stability in Water	N/A	N/A	No
Biodegradation	Yes	Yes	No
Fugacity	Yes	Yes	No
Ecotoxicity			
Acute Toxicity to Fish	Yes	Yes	No
Acute Toxicity to Aquatic Invertebrates	Yes	Yes	No
Acute Toxicity to Aquatic Plants	No	N/A	No
Animal Toxicity			
Acute Toxicity	Yes	Yes	No
Primary Irritation	Yes	Yes	No
Genotoxicity			
Point Mutation	Yes	Yes	No
Chromosomal Aberration	No	N/A	No
Repeat dose Toxicity	Yes	Yes	No
Reproductive Toxicity	No	N/A	No
Development and Teratogenicity Toxicity	No	N/A	No